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COMMUNICATION

# [*n*]Pseudorotaxanes constructed by a bis(*p*-phenylene)-34-crown-10-based cryptand: different binding behaviors induced by minor structural changes of guests

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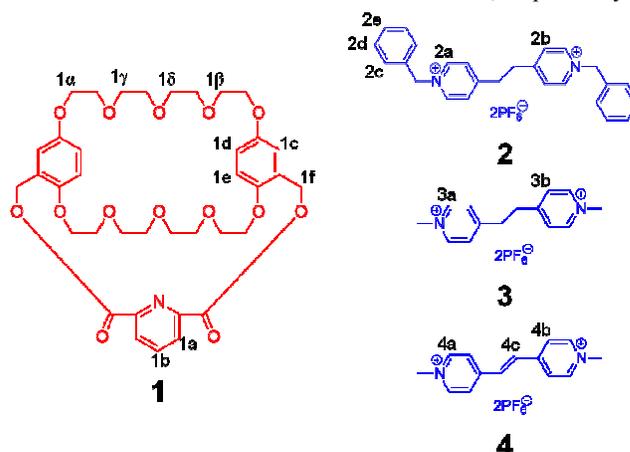
DOI: 10.1039/b000000x

Three pseudorotaxanes consisted of a bis(*p*-phenylene)-34-crown-10-based cryptand host and 1,2-bis(4-pyridinium)ethane/ethylene derivative guests were obtained. It was found that small structural changes on guests could have big effect on the binding behaviors of host–guest complexes.

In host–guest chemistry, threaded structures<sup>1</sup> have attracted a lot of attention not only because of their contributions in topology, but also due to their potential applications in artificial molecular machines, metal-organic frameworks, supramolecular polymers, nanotechnology, *etc.*<sup>2</sup> As the fundamental building blocks for fabricating advanced mechanically interlocked species with intriguing properties, pseudorotaxanes,<sup>3</sup> self-assembly complexes in which macrocyclic hosts encircle linear guests, play important roles in threaded structures and supramolecular chemistry. In general, minor structural changes on hosts or guests can cause large effects on binding behaviors and geometries of the resultant threaded structures, thereby influencing the formation of advanced supramolecular assemblies.<sup>4</sup> In view of [*n*]pseudorotaxanes, the same phenomena happen sometimes in many aspects, such as the stoichiometry, association constants, and so on.<sup>5</sup> Gibson *et al.* reported that association constants of pseudocryptand-type [2]pseudorotaxanes based on the self-assembly of bis(*m*-phenylene)-32-crown-10 pyridyl, quinolyl, and naphthyridyl derivatives with paraquat improve remarkably.<sup>6a</sup> Schalley and coworkers reported that the deslipping reaction of rotaxanes can be obviously caused by the simple exchange of a CH group by an isoelectronic *N* atom.<sup>6b</sup> Therefore, revealing the effect of structural changes on host–guest binding behaviors is very important and will promote the efficient construction of functional supramolecular materials.<sup>7</sup>

Vinylogous viologens, which were synthesized to modify and expand properties and functions of paraquats (due to their electrochemical and photochemical activities), were attractive building units for the preparation of pseudorotaxanes.<sup>8</sup> 1,2-Bis(4-pyridinium)ethane derivatives, as analogues of vinylogous viologens, have rarely been used to construct mechanically interlocked molecules, such as pseudorotaxanes and rotaxanes, possibly because of the lack of powerful hosts

which can recognize them efficiently.<sup>9</sup> Cryptands have been proved to be much more powerful hosts for organic salts than their crown ether precursors because of the introduction of additional binding sites and the preorganization of the host structures during the association process. Therefore, it is worthwhile to study the novel recognition motifs based on cryptands, vinylogous viologens, and their analogues. Herein, we reported three [*n*]pseudorotaxanes formed between bis(*p*-phenylene)-34-crown-10 (BPP34C10)-based cryptand **1** and 1,2-bis(4-pyridinium)ethane/ethylene derivatives (**2**, **3**, and **4**, Scheme 1). Though these three guests showed subtle differences in structures, the corresponding [*n*]pseudorotaxanes between cryptand **1** and them exhibited different host–guest binding behaviors and geometries in the solid state. By self-assembly of cryptand **1** and guest **2**, a [2]pseudorotaxane driven by hydrogen bonding and  $\pi$ – $\pi$  stacking interactions was formed in the solid state. Nevertheless, simply changing the benzyl groups in guest **2** to methyl groups afforded a [3]pseudorotaxane as shown by X-ray analysis. What is more, if the bridged ethyl chain in guest **2** was further replaced by an ethylene chain (guest **4**), the association constant between **1** and **4** increased about 465 and 128 times in acetone than those of **1**⊃**2** and **1**⊃**3**, respectively.



**Scheme 1** Chemical structures of BPP34C10-based cryptand **1** and 1,2-bis(4-pyridinium)ethane/ethylene derivatives **2**, **3**, and **4**.

Equimolar acetone solutions of cryptand **1** with viologens **2**,

3, and 4 were pale orange due to charge transfer interactions between the electron-rich aromatic rings of the host and the electron-poor pyridinium rings of the guests, which was a direct evidence for host-guest complexation. All of these three host-guest complexes were of 1:1 stoichiometry in solution as demonstrated by Job plots<sup>10</sup> (Figs. S2–S4, ESI†) based on UV-vis spectroscopy absorbance data in acetone. This was further confirmed by the electrospray ionization mass spectrometry (ESI-MS):  $m/z$  546.9 for  $[1\supset 2 - 2PF_6]^{2+}$  (Fig. S5, ESI†);  $m/z$  470.9 for  $[1\supset 3 - 2PF_6]^{2+}$  (Fig. S6, ESI†);  $m/z$  469.6 for  $[1\supset 4 - 2PF_6]^{2+}$  and  $m/z$  1084.0 for  $[1\supset 4 - PF_6]^+$  (Fig. S7, ESI†). Moreover, ESI-MS showed a single peak at  $m/z$  834.6 corresponding to  $[1_2\supset 3 - 2PF_6]^{2+}$  (Fig. S6, ESI†), indicating the [3]pseudorotaxane formation in gaseous phase.

By probing the charge transfer bands of the complexes by UV-vis spectroscopy and employing a titration method, the association constants ( $K_a$ ) were determined:  $4.65 (\pm 0.22) \times 10^2 M^{-1}$  for  $1\supset 2$  (Fig. S8, ESI†),  $1.69 (\pm 0.23) \times 10^3 M^{-1}$  for  $1\supset 3$  (Fig. S9, ESI†), and  $2.16 (\pm 0.21) \times 10^5 M^{-1}$  for  $1\supset 4$  (Fig. S10, ESI†), respectively. It was obvious that the  $K_a$  value of  $1\supset 4$  was much higher than those of  $1\supset 2$  and  $1\supset 3$ , which indicated that vinylogous viologen 4 was a stronger electron-acceptor than the viologen derivatives 2 and 3. Furthermore, the proton NMR spectra of equimolar (2.00 mM) acetone- $d_6$  solutions of cryptand 1 with guests 2 and 3 both displayed only one set of peaks, indicating fast-exchange complexation on the  $^1H$  NMR time scale (Fig. 1, spectra a–e). After complexation, protons  $H_{1a}$  and  $H_{1b}$  on host 1 shifted downfield, while  $H_{1c}$ ,  $H_{1d}$ , and  $H_{1e}$  on host 1 and  $H_{2b}$  on guest 2 shifted upfield. The proton NMR spectra of an equimolar (2.00 mM) acetone solution of 1 and 3 was also investigated and displayed similar chemical shift changes (Fig. 1, spectra a–c). However, compared with the spectrum of complex  $1\supset 4$  (Fig. 3a), only slight chemical shift changes were observed for the protons of guests 2 and 3, indicating that the binding affinity between host 1 and guest 4 is stronger than those of complexes  $1\supset 2$  and  $1\supset 3$ . These results were consistent with the association constants of these [n]pseudorotaxanes.

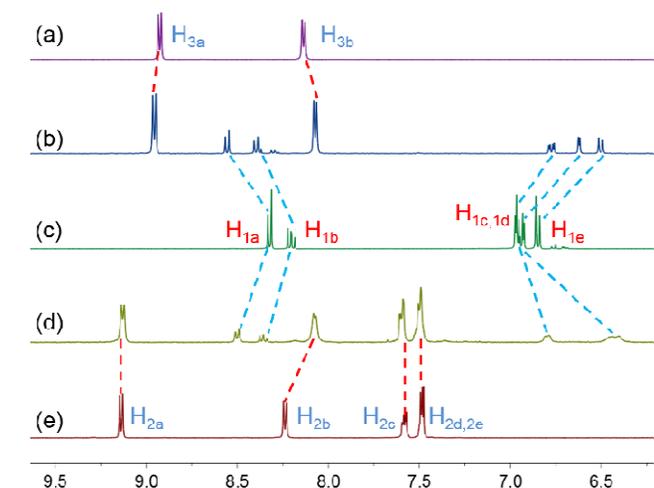


Fig. 1 Partial  $^1H$  NMR spectra (acetone- $d_6$ , 293 K, 400 MHz): (a) 2.00 mM 3; (b) 2.00 mM 3 + 2.00 mM 1; (c) 2.00 mM 1; (d) 2.00 mM 1 + 2.00 mM 2; (e) 2.00 mM 2.

With the purpose of further studying the host-guest complexation and the effects on the formation of [n]pseudorotaxanes caused by minor changes of the guests, a yellow crystal with 1:1 complexation stoichiometry between 1 and 2 was obtained *via* the vapor diffusion of diisopropyl ether into its acetonitrile solution. X-ray analysis of this crystal demonstrated that a [2]pseudorotaxane structure, stabilized by hydrogen bonds between the hydrogen atoms of 2 and ether oxygen atoms of 1, and  $CH\cdots\pi$  interactions, indeed formed between host 1 and guest 2 in the solid state (Fig. 2a). While for host-guest system between 1 and 3, X-ray diffraction analysis gave a strong evidence that a [3]pseudorotaxane structure was formed in the solid state (Fig. 2b). The complex is stabilized by twelve hydrogen bonds (h, i, j, k, l, and m), including four water bridge hydrogen bonds (k and j) between host 1 and guest 3, and face-to-face  $\pi$ -stacking between aromatic rings of 1 and 3. It is noteworthy that four hydrogen bonds (m and l) between the ether oxygen atoms of one host and the hydrogen atoms of the other host molecule formed, which favored the formation of a macrocyclic dimer structure. We reasoned that 1 and 2 did not form a [3]pseudorotaxane like  $1_2\supset 3$  (Fig. 2b) because the phenyl-substituted viologen derivative 2 appeared as a “zig-zag” shape after complexing with host 1, which prevented it to thread through the second host molecule. Furthermore, the  $CH\cdots\pi$  interaction (g) between 1 and 2 also helped to “hold” this [2]pseudorotaxane structure in the solid state.

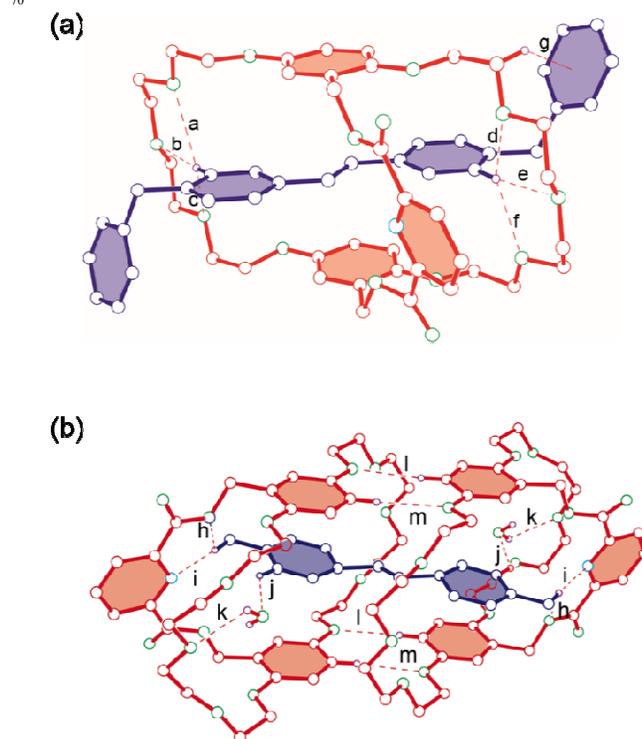
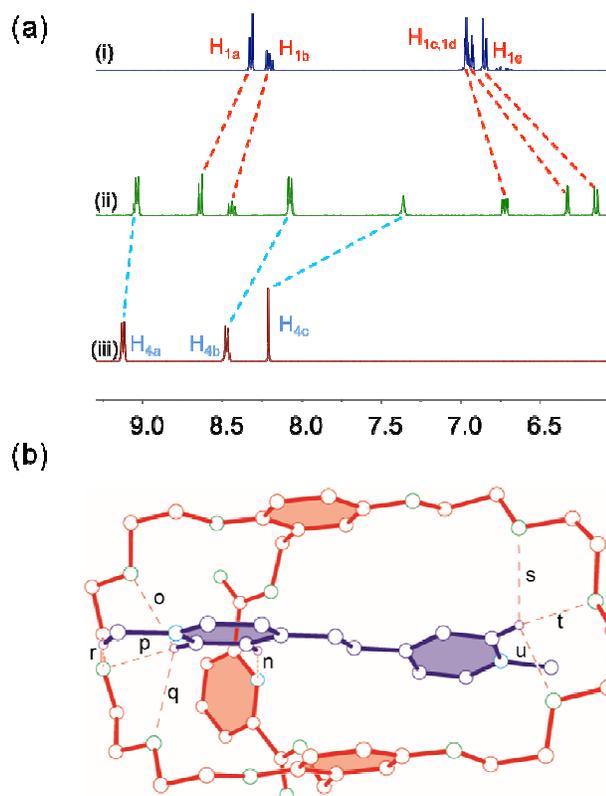


Fig. 2 Ball-stick views of X-ray crystal structures of (a)  $1\supset 2$  and (b)  $1_2\supset 3$ . Host 1 is red, guests 2 and 3 are blue, hydrogens are purple, oxygens are green, and nitrogens are sky blue.  $PF_6^-$  counterions and hydrogens except the ones involved in hydrogen bonding between 1 and 2 (or 3) were omitted for clarity. Hydrogen bond parameters are as follows: C $\cdots$ O (N) distance ( $\text{\AA}$ ), H $\cdots$ O (N) distance ( $\text{\AA}$ ), C(N)–

H...O (N) angles (deg): a, 3.17, 2.84, 101.5; b, 3.37, 2.45, 162.3; c, 3.17, 2.51, 126.7; d, 2.98, 2.44, 115.7; e, 3.19, 2.26, 164.0; f, 2.97, 2.67, 98.9; g, 3.69, 2.89, 138.9; h, 3.24, 2.64, 120.2; i, 3.43, 2.45, 174.6; j, 3.30, 2.58, 133.0; k, 3.16, 2.53, 132.0; l, 3.53, 2.59, 175.6; m, 3.54, 2.59, 175.7.

In order to clarify how small changes on guests influence the binding behavior of the  $[n]$ pseudorotaxanes, the complex  $1\supset 4$  was studied.  $^1\text{H}$  NMR spectra of an equimolar solution of host **1** and guest **4** showed that no signals corresponding to uncomplexed species were observed, indicating fast exchange on  $^1\text{H}$  NMR time scale (Fig. 3a). After complexation, peaks corresponding to  $\text{H}_{1\text{a}}$  and  $\text{H}_{1\text{b}}$  of host **1** shifted downfield, while  $\text{H}_{1\text{c}}$ ,  $\text{H}_{1\text{d}}$ , and  $\text{H}_{1\text{e}}$  of host **1** and  $\text{H}_{4\text{a}}$ ,  $\text{H}_{4\text{b}}$ , and  $\text{H}_{4\text{c}}$  of guest **4** moved upfield due to the shielding effect of the aromatic rings and electron density changes induced by the noncovalent interactions (H-bonding and charge-transfer interactions) between cryptand **1** and guest **4**, as we observed for  $1\supset 2$  and  $1\supset 3$ . A yellow crystal of  $1\supset 4$  was also grown by the same vapor diffusion method. It was interesting that the crystal structure of complex  $1\supset 4$  showed a  $[2]$ pseudorotaxane structure instead of a  $[3]$ pseudorotaxane structure in the solid state (Fig. 3b), although guest **4** was very similar to guest **3**. The possible reason is that guest **4** is a  $\pi$ -extended viologen derivative and possesses a much more rigid ethylene chain compared with the flexible ethyl chain in guest **3**, which facilitates the efficient charge-transfer interaction in a  $[2]$ pseudorotaxane-type threaded structure.



**Fig. 3** (a) Partial  $^1\text{H}$  NMR spectra (acetone- $d_6$ , 293 K, 400 MHz): (i) 2.00 mM **1**; (ii) 2.00 mM **1** + 2.00 mM **4**; (iii) 2.00 mM **4**. (b) Ball-stick views of X-ray crystal structure of  $1\supset 4$ . Host **1** is red, guest **4** is blue, hydrogens are purple, oxygens are green, and nitrogens are grey

blue.  $\text{PF}_6^-$  counterions and hydrogens except the ones involved in hydrogen bonding between **1** and **4** were omitted for clarity. Hydrogen bond parameters are as follows: C...O (N) distance ( $\text{\AA}$ ), H...O (N) distance ( $\text{\AA}$ ), C(N)-H...O (N) angles (deg): n, 3.58, 2.68, 159.7; o, 3.07, 2.55, 114.3; p, 3.32, 2.41, 159.8; q, 3.00, 2.65, 102.1; r, 3.55, 2.62, 157.5; s, 3.11, 2.60, 113.8; t, 3.20, 2.26, 154.4; u, 3.04, 2.63, 106.5.

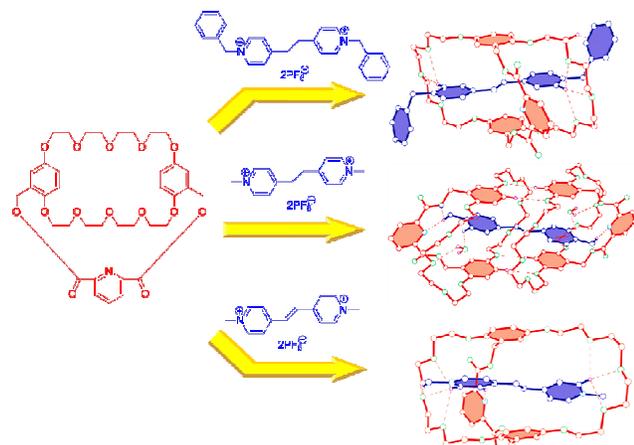
In summary, we studied the recognition of BPP34C10-based cryptand **1** to three 1,2-bis(4-pyridinium)ethane/ethylene derivatives (**2**–**4**) with minor structural differences. They revealed different association constants in solution and different binding behaviors and geometries in the solid state. By self-assembly of host **1** with guests **2** and **4**, the  $[2]$  pseudorotaxane-type threaded structures were formed in the solid state. However, the  $[3]$ pseudorotaxane-type host–guest complex  $1\supset 3$  was obtained in the solid state. The association constant values showed that guest **4** bound host **1** much stronger than guests **2** and **3**. These phenomena demonstrated that small structural or geometrical changes on guests could result in large effects on binding behaviors between hosts and guests, thereby leading to big differences in the configurations of the resulting  $[n]$ pseudorotaxanes. These different binding behaviors induced by small structure changes can be used to efficiently construct self-sorting system and further to fabricate more complex and highly ordered supramolecular materials with fascinating properties, distinct topologies, and novel function.

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## Notes and references

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- †Electronic Supplementary Information (ESI) available: determination of association constants, ESI-MS, X-ray crystallographic files (CIF) for  $1\supset 2$ ,  $1\supset 3$ , and  $1\supset 4$ , and other materials. See DOI: 10.1039/b000000x/
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**ToC Graphic:**

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**Text:**

Investigation on three pseudorotaxanes consisted of a bis(*p*-phenylene)-34-crown-10-based cryptand and three 1,2-bis(4-pyridinium)ethane/ethylene derivatives demonstrated that small structural changes on guests can greatly affect the host-guest binding behaviors.